

chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 14 15 16 17

chain bonds :

10-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 4-16 5-6 5-9 5-15 7-8 7-14 7-10 8-9 10-11

11-12 12-14 15-17 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-7 4-16 5-6 5-9 5-15 7-8 7-14 7-10 8-9 10-13

10-11 11-12 12-14 15-17 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

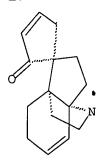
11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom

# L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7



Structure attributes must be viewed using STN Express query preparation.

=> s 17 full

FULL SEARCH INITIATED 20:11:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1251 TO ITERATE

100.0% PROCESSED 1251 ITERATIONS

SEARCH TIME: 00.00.01

IONS 34 ANSWERS

L8 34 SEA S

34 SEA SSS FUL L7

=> d 18 1-15

L8 ANSWER 1 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
RN 873078-37-6 REGISTRY
ED Entered STN: 31 Jan 2006
Spir(3)-cyclopeatene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
2,3-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (15,3'aS,5R,7'aS)(9C1) (CA INDEX NAME)
OTHER NAMES:
CN Dechlorodauricumine
FS STEREOSEARCH
MF C19 H25 N O6
ST CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 3 OF 34 REGISTRY COPYRIGHT 2007 ACS ON STN 637770-98-0 REGISTRY
Entered STN: 15 Jan 2004
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,4',5'-trione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
[1R,3'a5,5,7'a5,9's)- (9CI) (CA INDEX NAME)
STEREOSEARCH
C19 H22 C1 N 07
CA
STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 2 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 637770-99-1 REGISTRY
Entered STN: 15 Jan 2004
Spire(3-cyclopentene=1,10'-{3a,7a}propano{1H}indole]-2,5'{4'H}-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-6',7'-dimethoxy-1'-methyl-,
1R,3'aS,5R,7'aS,9'S)- (9CI) (CA INDEX NAME)
STEREOSEARCH
C18 H22 C1 N OS
CA
STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 4 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
637770-97-9 REGISTRY
ED Entered STN: 15 Jan 2004
CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-4,5',6',7'-tetramethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C20 H26 C1 N 06
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 5 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
637770-96-8 REGISTRY
Entered STN: 15 Jan 2004
Spiro[3-cyclopentene-1,10'-[3a, 7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-1'-ethyl-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,5'-oxime,
STEREOSEARCH
C20 H27 C1 N2 06

CA STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSVER 7 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 63770-94-6 REGISTRY
Entered STN: 15 Jan 2004
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-1'-ethyl-2',3'-dhydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)
CZO H26 Cl N O6
CA

CA
STN Files: CA, CAPLUS, USPATFULL

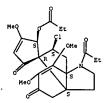
Absolute stereochemistry.

"PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT"

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSVER 6 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 637770-95-7 REGISTRY
  Entered STN: 15 Jan 2004
  Spire[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-5-(1-oxopropoxy)-1'-(1-oxopropoxy)-, (1R,3'a5,55,7'a5,9'S)- (9C1) (CA INDEX NAME)
  STEREOSEARCH
  C24 H30 C1 N O8
  CA
  STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



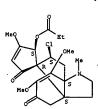
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- ANSWER 8 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 637770-93-5 REGISTRY
  Entered STN: 15 Jan 2004
  Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-1'-methyl-5-(1-охоргороху)-, STEREOSEARCH
  CZ2 H28 CIN 07
  CZ2 H28 CIN 07

- CA STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 9 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 488736-04-5 REGISTRY
Entered STN: 11 Feb 2003
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (15,3'aS,5R,7'aS)-STEREOSEARCH NAME)
STEREOSEARCH NAME)
C19 H25 N 06

STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 11 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
RN 486429-90-7 REGISTRY
ED Entered STN: 06 Peb 2003
CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-1-[3-(4-hydroxypheny1)-2-nitropropy1]-4,6',7'trimethoxy-, (15,3'a5,5R,7'a5,9'5)- (9CI) (CA INDEX NAME)
CTH RINTOTYRESAULTUMININE
FS STEREOSEARCH
HP C27 H31 C1 N2 08
SR CA
LC STN Files: C4

Absolute stereochemistry. Rotation (-). Currently available stereo shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 10 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN 488736-03-4 REGISTRY Entered STN: 11 Feb 2003 Spire(3-cyclopentene-1,10'-(3a,7a)propano[1H]indole]-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (15,3'a5,5s,7'a5)- (9CI) (CA INDEX NAME) STREGOSEARCH CL8 H23 N 06 CA

STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 12 OF 34 REGISTRY COPYRIGHT 2007 ACS ON STN
RN 345641-00-1 REGISTRY
ED Entered STN: 12 Jul 2001
Spir-[03-cyclopenten=-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1-methyl-,
(IR,3'as,5R,7'as,9'S)- (CA INDEX NAME)
OTHER NAMES:
CD Buricumine
STEREOSEARCH
HF C19 H24 C1 N O6
CA CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 ANSWER 13 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
RN 345640-99-5 REGISTRY
ED Entered STN: 12 Jul 2001
CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5' (4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'as,SR,7'as,9'S)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dauricumidine
FS STEREOSEARCH
HF C18 H22 C1 N O6
SR CA
LC STN Files: C'

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 15 OF 34 REGISTRY COPYRIGHT 2007 ACS on STN
RN 121255-00-3 REGISTRY
ED Entered STN: 23 Jun 1989
CN Spir-Gl3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
2',3'-dihydro-3,6',7'-trimethoxy- (9CI) (CA INDEX NAME)
CTHER CA INDEX NAMES:
CN Acutumine, 9-dechloro-12-demethoxy-1-demethyl-11-deoxy-13-methoxy-,
(105,155,165)CTHER NAMES:
CN (+)-Limalongine
CN Limalongine
MF C18 H23 N OS
SR CA
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAPLUS, NAPRALERT
('File contains numerically searchable property data)

Currently available stereo shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 14 OF 34 REGISTRY COPYRIGHT 2007 ACS ON STN
RN 219794-33-9 REGISTRY
ED Entered STN: 18 Feb 1999
CN Spir(c3)-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS)(SCI) (CA INDEX NAME)
OTHER NAMES:
CN Dechloroacutumine
FS STEREOSEARCH
HC C19 H25 N O6
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, TOXCENTER Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT'\*

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 201.35 385.83

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http://www.cas.org/infopolicy.html

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom
Stereo Bonds:
15-5 (Single Hash).
16-4 (Single Hash).
Stereo Chiral Centers:
     (Parity=Odd)
     (Parity=Odd)
Stereo RSS Sets:
Type=Relative (Default). 2 Nodes= 4 5
L10
       STRUCTURE UPLOADED
=> s 110 full
  REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

L12 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1053937 CAPLUS
DOCUMENT NUMBER: 145:460739
TITLE: 10nizing rule and characterist

145:460739 cule and characteristic spectra analysis of electrospray ionization for alkaloids in Menispermum daurtcum DC
Chen, Yong Chen, Huaixia
Hubei Province Key Lab. of Bio-Technology of Traditional Chinese Medicine, Hubei University, Wuhan, 430062, Peop. Rep. China
Penxi Ruawue (2006), 34(5), 675-678
CODEN: FRHDT7 ISSN: 0253-3820
Kewue Chubanshe

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

ISHER: Kexue Chubanshe
HSMT TYPE: Journal
UAGE: Chinese
The MS and MS2 spectra of tetrandrine and sinomenine in pos. ion detection
mode were analyzed by electrospray ionization quadrupole ion trap mass
spectrometry (ESI-QITMS), and their cleavage patterns were summarized.
The alkaloids extracted from the medicinal materials were also analyzed

The alkalous extlacted the model of the structure of the

Menispermun dauricum DC., were found in the extraction The characteristic print of

wen kinds of alkaloids (one has four kinds of isomers) in the standard medicinal materials was worked in selected ion monitor mode. 17088-50-5, Acutumine 18165-26-1, Acutumidine 22512-32-5, Acutuminine RL: ANT (Analyte); ANST (Analytical study) (anal. of alkaloids in Menispermum dauricum by electrospray ionization MS)

17088-50-5 CAPLUS

1/0e-30-3 CAPUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (IR,3'aS,5,7'aS,9'5)- (CA INDEX MAME)

Absolute stereochemistry.

18145-26-1 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

L12 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2006:1040729 CAPLUS DOCUMENT NUMBER: 146:54913 TITLE: Aporphine alkaloids and their

AUTHOR (S): CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

and their teversal of markets, and their flowes-of-CAPLUS

5piro(3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

# Absolute stereochemistry.

345641-00-1 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H]-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1-methyl-,
(1R,3'as,8',7'as,9's)- (CA INDEX NAME)

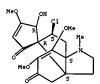
Absolute stereochemistry. Rotation (-).

L12 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN Absolute stereochemistry. Rotation (-).



23512-32-5 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H]-dione,9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,7'aS,9'S)-(9CI) (CA INDEX NAME)

L12 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT:

18 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L12 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:1228158 CAPLUS DOCUMENT NUMBER: 144:103959
TITLE: Dechlorodauricumine from cultu

Dechlorodauricumine from cultured roots of Menispermum

AUTHOR (5):

CORPORATE SOURCE:

Dechlorodauricumine from cultured roots of Menispern dauricum Sugimoto, Yukihiro; Hatsui, Miharu; Takikawa, Hirosato; Sasaki, Mitsuru; Kato, Hasako Graduate School of Science and Technology, Kobe University, Kobe, 657-8501, Japan Phytochemistry (Elsevier) (2005), 66(22), 2627-2631 CODEN: PTTCAS; ISSN: 0031-9422 Elsevier Ltd. SOURCE:

PUBLI SHER: DOCUMENT TYPE: English LANGUAGE:

DAGE: English
Dechlorodauricumine, a possible organic substrate for biochlorination, was isolated from cultured roots of Menispermum dauricum, a rich source of chlorinated alkaloids. Its structure was established by spectroscopic and

chlorinated alkaloids. Its structure was established by spectroscopi chemical methods.

17088-50-5P, Acutumine 345641-00-1P, Dauricumine RL: BSU (Biological study, unclassified), NPO (Natural product occurrence)) PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)

[alkaloid from roots of Menispermum dauricum]

17088-50-5 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

## Absolute stereochemistry.

345641-00-1 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1-methyl-, (1R,3'aS,5R,7'aS,9'S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

18145-26-1P, Acutumidine 345640-99-5P, Dauricumidine
RL: BSU (Biological study, unclassified): NPO (Natural product
occurrence): PERP (Purification or recovery): BIOL (Biological study): OCCU
(Occurrence): PERP (Preparation)
(alkaloid from roots of Menispermum dauricum)
18145-26-1 CAPLUS
Spiro(3-cyclopentene-1,10'-[3a,7a]propano{1H]indole}-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy'-4,6',7'-trimethoxy-,
(1R,3'a5,55,7'a5,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

345640-99-5 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'aS,5R,7'aS,9'S)- (9CI) (CA INDEX NAME)

# Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

219794-33-9P, Dechloroacutumine 873078-37-6P,
Dechlorodauricumine
RL: BSU (Biological study, unclassified); NPO (Natural product
occurrence); PRP (Properties); PUR (Purification or recovery); SFN
(Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP
(Preparation)
(alkaloid from roots of Menispermum dauricum)
219794-33-9 CAPLUS
Spirol3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

873078-37-6 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 2,3-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1S,3'aS,5R,7'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L12 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:559577 CAPLUS DOCUMENT NUMBER: 143:226001
TITLE: MORPHIAGE ...

143:226001

Morphinane Alkaloids with Cell Protective Effects from Sinomenium acutum
Bao, Guan-Huz Qin, Guo-Wei; Wang, Rui; Tang, Xi-Can Shanghai Institute of Materia Medica, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, 201203, Peop. Rep. China Journal of Natural Products (2005), 68 (7), 1128-1130 CODEN: JNPRDF; ISSN: 0163-3864
American Chemical Society
Journal English AUTHOR(S): CORPORATE SOURCE:

SOURCE:

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S):

MENT TYPE: Journal
JUNGE: English
RS SOURCE(s): CASREACT 143:226001
One new morphinane alkaloid, sinomenine N-oxide (1), and one new natural
occurring morphinane alkaloid, sinomenine N-oxide (1), and one new natural
occurring morphinane alkaloid, N-demethylsinomenine (2), together with six
known alkaloids, 7,8-didehydro-4-hydroxy-3,7-dimethoxymorphinan-6-ol (3),
sinomenine (4), sinoacutine (5), N-norsinoacutine, acutumine, and
acutumidine, were isolated from the stems of Sinomenium acutum. Their
structures were elucidated on the basis of spectroscopic anal, and chemical
methods. Compds. 2, 3, and 5 have protective effects against hydrogen
peroxide-induced cell injury.
17088-50-5P, Acutumine 18165-26-IP, Acutumidine
RL: BSU (Biological study, unclassified) NPO (Natural product
occurrence), PRP (Properties), PNE (Purification or recovery), BIOL
(Biological study), OCCU (Occurrence), PREP (Preparation)
(morphinane Alkaloids from Sinomenium acutum)
17088-50-5 CAPLUS
Spirol3-cyclopentene-1, 10'-[3a,7a]propano[IH]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(IR,3'as,55,7'as,9'S)- (CA INDEX NAME)

Absolute stereochemistry.



18145-26-1 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

REFERENCE COUNT:

21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
142:355429
Synthesis of the Core Structure of Acutumine
Reeder, Matthew D.; Srikanth, G. S. C.; Jones, Spencer
B.; Castle, Steven L.
Department of Chemistry and Biochemistry, Brigham
Young University, Provo, UT, 84620, UNIV. 84620

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

The tricyclic core of the bioactive natural product acutumine (I) has been synthesized. Key steps include an oxidative phenolic coupling to form a masked o-benzoquinone, an anionic oxy-Cope rearrangement to construct an all-carbon quaternary center, and a Michael-type cyclization to form an amine-bearing quaternary carbon. The target compound exists in solution as

ΙT

enol, in contrast to related compds. that are ketones. A model explaining these observations is presented.

17088-50-59
RL: PNU (Preparation, unclassified), PREP (Preparation)
(synthesis of the core structure of acutumine)

17088-50-5 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy'-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'as,5s,7'as,9's)- (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT REFERENCE COUNT:

L12 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2004:2861 CAPLUS DOCUMENT NUMBER: 140:59819
TITLE: Preparati 140:59819
Preparation and formulation of acutumine and acutumine compounds for the treatment of cognitive deficiency and neurodegenerative diseases (in, Guo-Weir Tang, Xi-Can, Lestage, Pierre; Caignard, Daniel-Henri; Renard, Pierre Shanghai Institute of Materia Medica, Peop. Rep. China: Les Laboratoires Servier FCT Int. Appl., 37 pp. CODEN: PIXXD2

INVENTOR (5):

PATENT ASSIGNEE(S):

Patent English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

F	PAT	ENT	NO.			KIN	D	DATE	:		APP	LICAT	ION	NO.		D	ATE			
٧	WO 2004000815				A1		2003		WO 2003-IB2600					20030616						
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB	, BG,	BR.	BY.	BZ.	CA.	CH.	CN.		
			co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC	, EE,	ES.	FI.	GB.	GD.	GE.	GH.		
			GM,	HR,	ΗU,	ID,	IL.	IN.	IS.	JP.	KE	, KG,	KP.	KR.	KZ.	LC.	I.K.	LR.		
			LS,	LT,	LU,	LV.	MA.	MD.	MG.	MK.	MN	, MW,	MX.	MZ.	NO.	NZ.	OM.	PH.		
			PL.	PT.	RO.	RU.	SC.	SD.	SE.	SG.	SK	, SL,	TJ.	TM.	TN	TR	TT	77		
			UA.	UG.	US.	UZ.	VC.	VN.	YU.	ZA.	2M	, 2W	,	••••	,	••••	,	,		
		RW:	GH.	GM.	KE.	LS.	MW.	M2.	SD.	SI.	57	, TZ,	uc	2M	7W	ΔМ	17	Dν		
			KG.	KZ.	MD.	RU.	TJ.	TM.	AT.	BE.	RG	CH,	CY,	C7	DF.	חצי,	EP.	DI,		
			FI.	FR.	GB.	GR.	HU.	IE.	TT.	LUL	MC	, NL,	PT.	BO.	SE.	SI.	CV.	TD,		
			BF.	BJ.	CF.	CG.	CT,	CM	GA,	GN,	GO	, GW,	MT.	MD,	NE.	eu,	Th.	TC,		
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	BB 2003012444				2.	A 20040100			BR 2003-12444						20030616					
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OTHER	50	URCE	(5):			MARI	'AT	140:	59819	•										

Acutumine and compds. thereof of formula I [R1, R2 = H, bond; R3 = H, alkoxy, R4 = H, OH, alkoxy, alkylcarbonyloxy, arylcarbonyloxy; R5 = H, halo; R6= H, alkyl, alkylcarbonyl, aroyl; R7, R10 = alkoxy; R8B3 = bond; R8R12 = sulfide bridge; R9R10 = oxo; R13 = H, C1; R11 = OH, alkoxy, oxo, oxime, O-alkyl oxime; R12 = H; with provisos] are prepared The compds. can be used for the treatment of cognitive deficiencies associated with cerebral ageing and with neurodegenerative diseases. Thus, II is prepared from acutumidine, formaldehyde and propanoic anhydride. II was shown to counteract scopolamine-induced memory impairments in the Horris water maze test in mice, indicating anti-ammesic properties.

23512-32-59
R1: PAC (Pharmacological activity); PIR (Purification or account of the complex of the

(Continued)

RE: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(isolation of acutumine compds. for the treatment of cognitive
deficiency and neurodegenerative diseases)
23512-32-5 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-1'-methy1-, (1R,3'as,7'as,9's)(SCI) (CA INDEX NAME)

Absolute stereochemistry.

637770-93-5P 637770-94-6P 637770-95-7P 637770-96-8P 637770-97-9P 637770-98-0P 637770-99-1P RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)

(preparation of acutumine compds. for the treatment of cognitive

(preparation of acutumine compose. 1.1.

deficiency
and neurodegenerative diseases)

837770-93-5 CAPLUS

CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-1'-methyl-5-(1-охоргороху)-,

(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 637770-96-8 CAPLUS
Spirc(3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-1'-ehtyl-2',3'-dthydro-5-hydroxy-4,6',7'-trimethoxy-,5'-oxime,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

637770-97-9 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-4,5,6',7'-tetramethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

637770-98-0 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,4',5'-trione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

637770-94-6 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H]-dione,
9'-chloro-1'-ethyl-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

637770-95-7 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-4,6',7'-trimethoxy-5-(1-cxopropoxy)-1'-(1cxopropy1)-, (1R,3'aS,55,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

637770-99-1 CAPLUS
Spiro(3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-6',7'-dimethoxy-1'-methyl-,
(1R,3'aS,5R,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 18145-26-1, Acutumidine
RL: RCT (Reactant): RACT (Reactant or reagent)
(preparation of acutumine compds. for the treatment of cognitive
deficiency
RN 18145-26-1
CAPLUS
CN Spiro(3-cyclopentene-1,10'-(3a,7a)propano[1H]indole]-2,5'(4'H)-dione,
9'-chioro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'as,55,7'as,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

17088-50-5P, Acutumine RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of acutumine compds. for the treatment of cognitive

(preparation of acutumine compos. For the treatment of cognitive deficiency and neurodegenerative diseases)

RN 17088-50-5 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 18145-26-1 CAPLUS
CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-),



219794-33-9 CAPLUS

219742-79clopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methy1-, (1R,3'a5,5s,7'a5)-(SCI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

488736-03-4P 488736-04-5P

488/36-03-4P 488/36-04-5P
RI: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
[4] Relation (1997) [4] Relat

Absolute stereochemistry. Rotation (-).

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI

The alkaloids, dechloroacutumidine (I) and 1-epidechloroacutumine (II), together with three known alkaloids, acutumidine, acutumine, and dechloroacutumine, were isolated from the rhizomes of Menispermum dauricum and their structures established by spectral and chemical methods. The cytotoxicity of each compound against the growth of human cell lines was studied, and acutumine selectively inhibited T-cell growth. 17088-50-5, Acutumine 18145-26-1, Acutumidine 218794-33-9, Dechloroacutumine RL: BSU (Biological study, unclassified), BIOL (Biological study) (alkaloids from Menispermum dauricum) 17088-50-5 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (18,3'a5,58,7'a5,9'S)- (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



488736-04-5 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1s,3'aS,SR,7'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
138:112112
Nitrotyrasacutuminine from Henispermum dauricum
Yu, Bing-Wuy Chen, Jian-Yongy Zhou, Tian-Xi; Cheng,
Kin-Fair Qin, Guo-Wei
Schneges Sciences, Shanghai Institutes of Hateria Hedica, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, 200031, Peop. Rep. China
Natural Product Letters (2002), 16(3), 155-159
CODEN: NPLEEF; ISSN: 1057-5634
Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nitrotyrasacutuminine, an unusual nitrated morphine-type alkaloid was isolated from the roots of Menispermum dauricum. Its structure was determined

rmined
by various 2D spectra and chemical methods.
486429-90-7P, Nitrotyrasacutuminine
RL: NPO (Natural product occurrence): PUR (Purification or recovery): THU
(Therapeutic use): BIOL (Biological study): OCCU (Occurrence): PREP
(Preparation): USES (Uses)
(nitrotyrasacutuminine from Henispermum dauricum)
486429-90-7 CAPLUS
Spirol3-cyclopentene-1, 10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-1-[3-(4-hydroxypheny1)-2-nitropropy1]-4,6',7'trimethoxy-, (15,3'a5,5R,7'as,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Currently available stereo shown.

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

18145-26-1 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'a5,5,7'a5,9')- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

345640-99-5P 345641-00-1P

Notes of the Properties of the

(cnfortnated atkalolus in Henispermum dauricum root culture and st in their formation) 345640-99-5 (CAPUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (IR,3'a5,8,7'a5,9'5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L12 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:268660 CAPLUS
DOCUMENT NUMBER: 135:58490
TITLE: Chlorinated alkaloids in Menispermum dauricum DC. root

Culture
Sugimoto, Yukihiro; Babiker, Hind A. A.; Saisho,
Tomoki; Furumoto, Toshio; Inanaga, Shinobu; Kato, AUTHOR (S):

CORPORATE SOURCE:

Tomoki, Furumoto, Toshio; Inanaga, Shinobu; Kato, Masako Arid Land Research Center, Tottori University, Tottori, 680-0001, Japan Journal of Organic Chemistry (2001), 66(10), 3299-3302 CODEN: JOCEAH; ISSN: 0022-3263 Americ SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

Faeding expts. using 36Cl showed that Menispermum dauricum root culture produces four alkaloids containing chlorine. They included the novel alkaloids dauricumine (1) and dauricumidine (11) as well as the known alkaloids acutumine and acutumidine. The structures of novel alkaloids were established by spectroscopic, crystallog, and chemical methods. Thes four alkaloids were labeled with 36Cl, isolated, and fed independently to root cultures. Mutual conversion between acutumine and acutumidine, and between dauricumine and dauricumidine by N-methylation and N-demethylation, was demonstrated. Moreover, dauricumine was converted to acutumine and acutumidine. Epimerization of acutumidine to dauricumidine or vice Versa was not observed These results suggest that dauricumine is

first chlorinated alkaloid formed in cultured M. dauricum roots. Skewed distribution of radioactivity derived from labeled dauricumine is proof that epimerization at C-1 proceeds at a lower rate than N-demethylation. 17088-50-5 18145-26-1
RL: BOC (Biological occurrence), BPR (Biological process); BSU (Biological study, unclassified), MFM (Metabolic formation), BIOL (Biological study); FORM (Formation, nonpreparative), OCCU (Occurrence), PROC (Process) (chlorinated alkaloids in Menispermum dauricum root culture and study in their formation)

in their formation)
1788-50-5 (APJUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloroc'2,3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(IR,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

345641-00-1 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1-methyl-, (IR,3'a5,5R,7'a5,9'5)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1999:243783 CAPLUS DOCUMENT NUMBER: 131:29875

131:29875
Biodynthetic relationship between acutumine and dechloroacutumine in Menispermum dauricum root cultures
Babiker, Hind A. A.; Sugimoto, Yukihiro; Saisho, Tomoki; Inanaga, Shinobu; Hashimoto, Masayuki; Isogai, Akira AUTHOR (S):

Akira

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

HOR(S):

Babiker, Hind A. A.; Sugimoto, Yukihiro; Saisho, Tomoki; Inanga, Shinobu, Hashimoto, Masayuki; Isogai, Akira

PORATE SOURCE:

Arid Land Research Center, Tottori University, Tottori, 680-0001, Japan
Bioscience, Bioscchology, and Biochemistry (1999), 63(3), 515-518

CODEN: BBBES; ISSN: 0916-8451

Japan Society for Bioscience, Biotechnology, and Agrochemistry

UNENT TYPE:

UNENT TYPE:

UNENT TYPE:

UNENT TYPE:

UNENT TYPE:

UNENT TYPE:

Journal

GUAGE:

The biosynthetic relationship between acutumine (I) and dechloroacutumine (II) was studied by using 13C-labeled tyrosine and 3H-labeled 2 as tracers. 13C-NHR spectra of 13C-labeled tyrosine and 3H-labeled 2 as tracers. 13C-NHR spectra of 13C-labeled tyrosine and 3H-labeled 7 coots, outlured in a chloride-enriched medium, with 3H-labeled II demonstrated that I is the only alkaloid metabolite of II. Conversion (54) of the exogenously applied II, taken up by the roots, into I showed that II is the precursor of I. Incomplete conversion of II into I suggests accumulation of the encymes involved in the biosynthesis of I. 219794-33-9. Dechloroacutumine

RL: BPR (Biological process) BSU (Biological study, unclassified), MFM (Metabolic Cormation), BIOL (Biological study), FORM (Formation, nonpreparative); PRCC (Process)

(Biosynthetic relationship between acutumine and dechloroacutumine in Meniapermum dauricum root cultures)

219794-33-9 CAPIUS

Spirol3-cyclopentene-1,10'-(3a, 7a)propano(1H)indole)-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (IR,3'as,55,7'as)-colute stereochemistry. Rotation (-).

Absolute stereochemistry. Rotation (-).

17088-50-5, Acutumine
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative) (biosynthetic relationship between acutumine and dechloroacutumine in Meniappermum dauricum root cultures)
17088-50-5 CAPLUS

L12 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:227389 CAPLUS
DOCUMENT NUMBER: 131:4278
ITILB: Effects of chloride ion on acutumine and dechloroacutumine production by Menispermum dauricum root culture
AUTHOR(S): Babiker, H. A. A.; Sugimoto, Y.; Saisho, T.; Inanaga,

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE:

HOR(S):
Babiker, H. A. A.; Sugimoto, Y.; Saisho, T.; Inanaga, S.
PORATE SOURCE:
Arid Land Research Center, Tottori University, Tottori, 680-0001, Japan
RCE:
Phytochemistry (1999), 50(5), 775-779
CODEN: PYTCAS; ISSN: 0031-9422
LISHER:
Lisevier Science Ltd.
MENT TYPE:
Journal
SUAGE:
English
The effects of chloride ion on the production of acutumine and dechloroacutumines by Menispermum dauricum root culture, were studied.
The chloride ion content in the medium plays a key role in the production of both alkaloids. A low chloride medium promoted production of dechloroacutumines and suppressed that of acutumine. Production of the two alkaloids during the 60 day culture period was closely associated with root biomass. Both alkaloids accumulated in the roots and a relatively small proportion was exuded into the medium. The intact plant produced very low amts. of both alkaloids. On the average, cultured roots contained 22 and 75-fold more acutumine and dechloroacutumine, resp., than intact plants.
17088-50-5P, Acutumine 219794-33-9P, Bechloroacutumine
RL: MHF (Bioindustrial manufacture); BPR (Biological process); BSU (Biological study, unclassified) BIOL (Biological study): PREP (Preparation); PROC (Process)
(effects of chloride ion on acutumine and dechloroacutumine production by Menispermum dauricum root culture)
17088-50-5 CAPIUS
Spirol3-cyclopentene-1, 10'-[3a, 7a] propano([H] indole]-2,5' (4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, Clut stereochemistry.

# Absolute stereochemistry.

219794-33-9 CAPLUS Spiro(3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methy1-, (1R,3'as,5s,7'as)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 10 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H]-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1998:785030 CAPLUS DOCUMENT NUMBER: 130:122231

TITLE: Dechloroacutumine from cultured roots of Menispermum

AUTHOR (5):

dauricum
Sugimoto, Yukihiro; Inanaga, Shinobu; Kato, Hasako;
Shimizu, Toshiyuki; Hakoshima, Toshio; Isogai, Akira
Arid Land Research Center, Tottori University,
Tottori, 680-0001, Japan
Phytochemistry (1998), 49(5), 1293-1297
CODEN: PYTCAS; ISSN: 0031-9422
Elsevier Science Ltd.
Journal CORPORATE SOURCE:

SOURCE:

PUBLI SHER:

DOCUMENT TYPE: LANGUAGE:



A novel alkaloid, dechloroacutumine (I), was isolated from Menispermum dauricum roots, a rich source of the chlorine-containing alkaloid acutumine cultured in chlorine-deficient medium. Its structure was elucidated by spectral and crystallog, anal. 219794-33-9P, Dechloroacutumine RL: BOC (Biological occurrence): RSU (Biological study, unclassified): PRP (Properties): PUR (Purification or recovery): BIOL (Biological study): OCCU (Occurrence): PREP (Preparation) (dechloroacutumine from cultured roots of Menispermum dauricum) 219794-33-9 CAPUS

219/94-35-9 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS)-(9C) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

L12 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:
DOCUMENT NUMBER:
1997:279419 CAPLUS
127:31581
Effect of 7-450 inhibitors on benzylisoquinoline
alkaloid biosynthesis in cultured roots of Stephania
cepharantha and Menispermum dauricum
scepharantha and Menispermum dauricum
lsogai, Akira
CORPORATE SOURCE:
SUBRICE:
SOURCE:
FUBLISHER:
PUBLISHER:
PUBLISHER:
DOCUMENT TYPE:
DOCUMENT TYPE:
JOURNAIL
English
English

DOCUMENT TYPE: LANGUAGE:

MENT TYPE: Journal
UAGE: English
The effect of cytochrome P 450 inhibitors was studied on biosynthesis of
benzylisoquinoline alkaloids, in cultured roots of S. cepharantha and M.
dauricum. In S. cepharantha only 2 alkaloids, aromoline and berbamine,
were produced. Most inhibitors reduced root growth and alkaloid
biosynthesis. Aromoline and berbamine contents were pos. correlated with
root growth. In M. dauricum anoymidol and metyrapone promoted root
growth, ketoconazole was inhibitory, while other inhibitors had
inconsistent effects. Production of the alkaloids dauricine and acutumine

curtailed by all inhibitors. Alkaloid contents were not related to root growth. None of the inhibitors induced accumulation of the immediate monomeric precursors of bis-benzylisoquinoline. Ketoconazole-treated M. dauricum roots accumulated tyramine, an early precursor of benzylisoquinoline, and 2 unidentified Tyr-derived alkaloids with mol. masses of 353 and 426.
17088-50-5P, Acutumine
RL: BOC (Biological occurrence); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(450 inhibitors effect on benzylisoquinoline alkaloid biosynthesis in cultured roots of Stephania cepharantha and Menispermum dauricum)
17088-50-5 CAPUIS
Spirol3-cyclopentene-1;10'-(3a, 7a]propano[1H] indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'as,55,7'as,9'S)- (CA INDEX NAME)

ΙT

Absolute stereochemistry.

L12 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1996:198363 CAPLUS DOCUMENT NUMBER: 124:255828 Early steps of dauricine biosyr

124:255828
Early steps of dauricine biosynthesis in cultured roots of Henispermum dauricum.
Sugimoto, Yukihiro; Uchida, Shinji; Inanaga, Shinobu; Kimura, Yasuo; Hashimoto, Masayuki; Isogai, Akira Arid Land Research Center, Tottori University, Tottori, 680, Japan Bioscience, Biotechnology, and Biochemistry (1996), 60(3), 503-5
CODEN: BBBIEJ; ISSN: 0916-8451
Japan Society for Bioscience, Biotechnology, and Agrochemistry
Journal AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

When Type:

Journal

UAGE:

Cultured roots of M. dauricum, were fed with L-[U-14C] tyrosine,
L-[3-13C] tyrosine, and [2-13C] tyramine independently, and the
incorporation of possible early precursors into dauricine (I) was studied.
I was composed of four mols. of tyrosine, and tyramine was specifically
incorporated into the isoquinoline portions of I. Acutumine, into which
I4C-labeled tyrosine was also incorporated, was identified as one of the
main constituents in the alkaloid fraction from the roots.

RL: BSU (Biological study, unclassified), HFM (Metabolic formation), BIOL
(Biological study), FORM (Formation, nonpreparative)

[1088-50-5 CAPLUS

Spiro[3-cyclopentene-1,10'-[3a,7a] propano[1H] indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydrosy-4,6',7'-trimethoxy-1'-methyl-,
(IR,3'as,5s,7'as,9's)- (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:547845 CAPLUS
DOCUMENT NUMBER: 101:147845
TITLE: 150lation of (-)-stepholidine, an alkaloid of
antiserotonergic-like activity from Sinomenium acutum
AUTHOR(S): Ichikawa, Kazuo, Kinoshita, Takeshir Itai, Akiko)
Iitaka, Yolchir Sankawa, Ushio
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: HTCYMM, ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A tetrahydroprotoberberine alkaloid, (-)-stepholidine, was isolated as an
active principle showing antiserotonergic-like activity from S. acutum
(Menispermaceae) which has been used as an oriental medicinal drug
(Japanese name, Bohi; Chinese name, Fang-Ji) in Japan. An aporphine type
alkaloid, liriodenine, was isolated first time from this plant along with
known alkaloids hitherto obtained from this plant.
IT 17088-50-5
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

17088-50-5
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
BIOL (Biological study); OCCU (Occurrence)
(of Sinomenium acutum)
17088-50-5 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

### Absolute stereochemistry.

L12 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:548475 CAPLUS
DOCUMENT NUMBER: 75:148475
TITLE: Alkaloids from Menispermum canadense
DOSACCE, RAYMOND W., Knapp, Joseph E.
CORPORATE SOURCE: Coll. Pharm. Ohio State Univ., Columbus, OH, USA
SOURCE: LLOYALS (1971), 34(3), 292-300
CODEN: LLOYALS (1971), 34(3), 2

# Absolute stereochemistry.

18145-26-1 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (1R,3'a5,5S,7'a5,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:500745 CAPLUS

DOCUMENT NUMBER: 89:100745

Search for inhibitors of microorganisms among the alkaloids

AUTHOR(S): Search for inhibitors of microorganisms among the alkaloids

Vichkanova, S. A.; Adgina, V. V.; Izosimova, S. B.;

Shipulina, L. D.; Lyutikova, L. I.

CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Lek. Rest., Bittsa, USSR

Khimiko-Parmatsevticheskii Zhurnal (1978), 12(2), 101-7

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The inhibitory activity of >30 alkaloids against microorganisms and viruses was determined Marked antimicrobial activity was observed with compds.

viruses was determined Marked antimicrobial activity was observed with compds.

such as nuphleine-HCl [25249-43-8], lutenurine [63937-19-9], sanguinarine sulfate (22331-93-7], and chelerythrine [34316-15-9] whose active concns. against Staphylococcus aureus were 0.24-7.8 µg/mL. Most of the 30 alkaloids and alkaloid prepns. tested against viruses were active, with chelidonine sulfate [66723-59-9] and 0-acetylchelidonine-HCl [66723-62-4] showing particularly marked activity.

17 66723-62-4

RL: BAC (Biological activity or effector, except adverse), BSU (Biological study, unclassified), BIOL (Biological study)

(virucidal activity of (Singuish) (Virucidal activity)

(Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, hydrochloride, [3'as-[3'as,7'aa,9'R\*,10'5\*(R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L12 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) L12 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1971:449368 CAPLUS COPYRIGHT 2007 ACS ON STN 75:49368

75:49368
Alkaloids of menispermaneous plants. CCLIX.
Alkaloids of Menisperman dauricum. Structures of acutumidine, chlorine-containing alkaloids with a novel skeleton Tomita, Masaon Okamoto, Yasukor Kikuchi, Tohrur Osaki, Kenjin Nishikawa, Masaon Kamiya, Kazuhider Sasaki, Yoshior Matcha, Katsuhider Goto, Kakuji Kyoto Coll. Pharm. Kyoto, Japan Chemical & Pharmaceutical Bulletin (1971), 19(4), 770-91

AUTHOR (S):

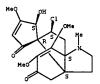
CORPORATE SOURCE:

DOCUMENT TYPE:

LANGUAGE:

Chemical & Pharmaceutical Bulletin (1971), 19(4),
770-91
CODEN: CPBTAL, ISSN: 0009-2363
GUAGE: Brights Journal
GUAGE: Brights Structures of acutumine (I) and acutumidine (II), isolated from M.
dauricum DC. and Sinomenium acutum Rehd. at Wils. (Menispermaceae), were
investigated. On the basis of degradative and spectroscopic evidence,
their structures in and II which agreed with the x-ray anal. These alkaloids
represent a new class of alkaloids with a novel skeleton and also provide
examples of Cl-containing alkaloids.
33110-49-59 33381-24-7P
RL: SPN (Synthetic preparation), PREP (Preparation)
(preparation of)
33110-49-5 CAPLUS
Spiro(3-cyclopentene-1, 10'-(3a, 7a)propano(1H) indole)-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-bhydroxy-4,6',7',-'t-rinenbony-1'-methy1-,
hydrobromide, [3'as-[3'aa,7'aa,9'R\*,10'5\*(R\*)]}- (9CI) (CA)

### Absolute stereochemistry.



### • HBr

33381-24-7 CAPLUS Sjrc[3-cyclopenten=1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
monooxime, {3'aS-[3'aa,7'aa,9'R\*,10'S\*(R\*)]]- (9CI) (CA INDEX
NAME)

CH 1

CRN 17088-50-5

L12 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN CHF C19 H24 C1 N O6 (Continued)

CM 2

CRN 7803-49-8 CMF H3 N O

## н2№- он

17088-50-5 18145-26-1
RL: PRP (Properties)
(structure and configuration of)
17088-50-5 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)



18145-26-1 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
(1R,3'as,5S,7'as,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1971:1113 CAPLUS COPYRIGHT 2007 ACS ON STN 74:1113 TITLE: Albertage Alberta

Alkaloids of Menispermaceous plants. CCLVIII. Alkaloids of Menispermum dauricum. Basic components of Siberian Menispermum dahuricum (Lunosemyannik daurskii)

Gaurakii; Tomita, Masao; Okamoto, Yasuko; Nagai, Yoshiko; Tanaka, Shigeko; Hayata, Toshie Kyoto Coll. Pharm., Mukogawa Women's Univ., Kyoto, AUTHOR (S):

CORPORATE SOURCE:

DOCUMENT TYPE:

FORATE SOURCE: Kyoto coll. Pharm., Mukogawa Women's Univ., Kyoto, Japan
RCE: Yakugaku Zasshi (1970), 90(9), 1182-6
CODEN: YXKZAJ, ISSN: 0031-6903
UMENT IYPE: Journal Of The Structurally Known
Japanese
For diagram(s), see printed CA Issue.
From the rhizome of the Russian M. dauricum, the structurally known
stepharine, acutumidine, magnoflorine, and a new biscoclaurinetype base,
dauricinoline (I), were newly isolated besides dauricine, sinomenine,
acutumine, and menisperine already reported in literature. I occurs as a
pale yellow powder and its methylation with diazomethane gives
o-methyldauricine. The O,O-di-Et compound, obtained by ethylation with
diazoethane, undergoes fission by metallic Na in liquid NH3 and produces
D-1-[P-ethoxybenzy]-6-ethoxy -7-methoyr-2-methyl-1,2,3,4tetrahydroisoquin-oline as the nonphenolic base and D-armepavine as the
phenolic base. From these results, the structure of I is as shown.
18145-26-1
RL: BOC (Biological occurrence), BSU (Biological study, unclassified),
BIOL (Biological study); OCCU (Occurrence)
(of Menispermum dauricum)
18145-26-1 CAPUIS
Spirol3-cyclopentene-1,10'-{3a,7a}propano[lH]indole}-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
[1R,3'as,5s,7'as,9's)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:450281 CAPLUS

DOCUMENT NUMBER: 71:50281

AUTHOR(S): Acutuminine, new alkaloid from the leaves of Menispermum dauricum

OKAMOTO, Yasukor Yuge, Etsukor Nagai, Yoshikor Katsuta, Riekor Kishimoto, Atsukor Kobayashi, Yoshikor Kikuchi, Tohrus Tomita, Masao

Fac. Pharm. Sci., Mukogawa Vomen's Univ., Nishinomiya, Japan

SOURCE: Tetrahedron Letters (1969), (24), 1933-5

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Isolation from the leaves of M. dauricum gave together with sinomenine, acutumine, disinomenine and stepharine, a small amount of a new crystalline alkaloid, acutuminine (I), m. 175-7.5°, (a)D -100°

(CHCI3). N.H.R., ir, uv, and mass suggested the structure for 1.

II 23512-32-5

RLI RCT (Reactant); RACT (Reactant or reagent)

(new alkaloid from Menispermum dauricum, structure of)

RN 23512-32-5 CAPLUS

ON Spiro[3-cyclopentene-1,10°-[3a,7a]propano[1H]indole]-2,5°(4'H)-dione, 9°-chloro-2',3°-dihydro-4,6°,7°-trimethoxy-1'-methyl-, (1R,3°aS,7°aS,9°S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
DOCUMENT NUMBER:
DOCUMENT NUMBER:
DOCUMENT NUMBER:
SOURCE:
AUTHOR(S):

SURCE:

SURCE:

DOCUMENT TYPE:
Journal
LANGUAGE:
AB The structures of acutumine and acutumidine
SOURCE Brown and (a)D -212 (pyridine), and acutumine (II),
isolated from Sinomenium acutum or Henispermum dauricum, were established.
The reduction of II acetate with LiAllHig gave a demethoxy dihydroxy ketone
(III), m. 136-7'. Treating II with Zn in boiling Ac20 gave a mixture
of IV (RI = R4 - Ac, R2 - H, R3 - MeO, IVA) and IV (RI = R4 - Ac, R2 Cl, R3 - H) (IVb). IVA was hydrolyzed, giving a phenolic compound, which
was methylated with CH2R2, giving IV (RI - R2 - H, R3 - MeO, R4 - He)
(IVc). IVC was treated with Ac20 in pyridine, giving IV (RI - Ac, R2 - H,
R3 - MeO, R4 - Me), and also oxidized with MnO2, giving the ene-dione
compound (V), m. 184-6'. The Whood oxidation of IV cgave a product, m.
75-7'', which was identified as 4,5,6-trimethoxy-1-indanone. Mild
saponification of IVb, followed by Wenlow at boundt to
colored by Whood oxidation, a compound m, 92-6', which was the athout to
colored by Whood oxidation, a compound m, 92-6', which was the athout to
colored by Whood oxidation, a compound m, 92-6', which was the pathought to

cl, Ne amb), m. 219-21.5' (decomposition), which gave, on LiAlH4 reduction followed by MAnO4 oxidation, a compound m. 92-6', which was thought to be 4,6-dimethoxy-1-indanone. The reduction of II with Zn-AcOH gave a dihydro

18145-26-1 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-,
{1R,3'aS,5S,7'aS,9'S}- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 21 OF 28
ACCESSION NUMBER:
DOCUMENT NUMBER:
1968:431127 CAPLUS
69:31127
The x-ray analyses of acutumine and its acetate; a trial of a short cut in the structure elucidation
Nishikawa, Masaor Kamiya, Kazuhide; Tomita, Masao;
Okamoto, Yasukor Kikuchi, Tohrur Osaki, Kenjir Tomite,
Yujiro; Nitta, Isamu; Goto, K.
Res. Develop. Div., Takeda Chem. Ind., Ltd., Osake,
Japan
SOURCE:
Journal of the Chemical Society [Section] B: Physical
Organic (1968), (6), 652-8
CODEN: JOSPAC, ISSN: 0045-6470
JOURNAL TYPE:
JOURNAL BENGLAME
AB The crystal and mol. Structures of acutumine, a novel type of alkaloid

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The crystal and mol. structures of acutumine, a novel type of alkaloid
containing Cl, and of its acetate, have been solved by x-ray anal. by using

three-dimensional Patterson superposition method and repeated application of least sqs. and three-dimensional Fourier methods. The result agreed with the chemical evidence obtained by concurrent degradative studies. The structure of acutumine is closely related to that of hasubanonine which was isolated from a species of the same plant family, but has a spirantype juncture of the five-membered rings A and B, with a Cl atom attached to the latter. The usefulness of applying the least-sqs. method at an unusually early stage for distinguishing real atoms from the spurious peaks appearing in the maps of min. functions or of Fourier synthesis was clearly demonstrated. In particular, observation of the behavior of erature

clearly demonstrated. In particular, observation of the Denavior of temperature factors through several cycles of least-sqs. with fixed atomic coordinates was found to provide a rapid method.

IT 17088-50-5
RI: PRP (Properties)
(structure of, calon. of, short method for)
RN 17088-50-5 CAPLUS
CN Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'as,5S,7'as,9'S)- (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L12 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1967:517002 CAPLUS

67:117002 GAPLUS

67:117002 ACULUMING, chlorine-containing alkaloids with a novel skeleton. II. Chemical proof Tomita, Masson Okamoto, Yasukor Kikuchi, Tohruv Osaki, Kenji, Nishikawa, M.; Kamiya, Kazuhider Sasaki, Yukio; Matoba, Katsuhider, Goto, Kaku, Katsuhider, Goto, Taku, Copyrona (Copyrona)

50URCE: SOURCE: 10507, (25), 2425-30 CODEN: TELEAY, ISSN: 0040-4039

DOCUMENT TYPE:

DOCUMENT TYPE: LANGUAGE:

COENT: TELEAY; ISSN: 0040-4039

UMENT TYPE: Journal

GUAGE: English

For diagram(s), see printed CA Issue.

cf. preceding abstract Based on previously reported exptl. evidence (CA 67: 54324k) and addnl. findings, 3 partial revised structures for acutumine are proposed (1, 11, 11). Acutumine (1V, R = Me, R = H) (V) has a tetrasubstituted 6-membered o, β-unsaid. Acutumine acceptage on or two MeO groups at the a,β positions. Acutumine acceptage on or two MeO groups at the a,β positions. Acutumine acceptage to the structure; I v has a secondary allyl alc. system. Treatment of VI with NaBMH gave a hydroxy compound (VII), showing a pos. Cotton effect at 304 mg. The ir absorption at 1690 cm.-1 and the uv band at 245 mg in various acutumine derivs. were accordingly ascribed to a hindered five-membered conjugated ketone system. Reduction of VI with LiAllid gave a dimethoxy-dihydroxy ketone (VIII), m. 136-7°, showing a pos. Cotton effect. Oxidation of V with MnO2 gave a dehydro product (IX), v 1745, 1695 cm.-1, indicative of a 5-membered ene-dione system. The above evidence supported the partial structure III The partial structure III followed mainly from N.H.R. spectral evidence. Treatment of V with Zn in boiling Ac20 gave a mixture containing a neutral fraction consisting of 2 aromatic N-free products, mainly (X, Rl = R2 = Ac) (XI), which hydrolyzed gently to give a phenolic compound which methylated with CH2N2 to an O-methyl ether X (Rl = Me, R2 = H) (XII), and acctylated with Ac20-CSHSN to the accetate X (Rl = Me, R2 = Ac) (XIII). The N.H.R. spectra of XI, XII. XIII indicated that the partial structure II proposed for V might remain unchanged in these products. MnO2 oxidation of XII gave an ene-dione (XIV), m. 154-6°. XII oxidized with RMnO4 gave a product, m.

73-7°, identified as 4,6,6-trimethoxy-1-indanone. The minor degradation product (VX, Rl = R2 = Ac) saponified and methylated gave an O-methyl ether XV (Rl = Me, R2 = H), m. 219-0-21.5° (decomposition), which reduced with LiAllid and consequently oxidized with

accordingly expanded to the partial structure (XVI) and the remaining moiety (C3H7N) was considered to form a -CH2CH2NMe- grouping based on N.M.R. study. Reduction of V with Zn-AcOH gave a dihydro compound (XVII),

m.

168-71°. Acetylation expts. suggested that XVII is most likely a carbinolamine, formed by cyclization of the normal reduction product (XVIII).

The circular dichroism curves of V and acutumidine IV (R = Rl = H) have a neg. Cotton effect near 320 mμ, attributed to the n → π° transition of a 6-membered α,β-unsatd. ketone system, comparable to the Cotton effect of hasubanonine (XIX) with the same structural feature of established configuration, thus establishing the structures of acutumine and acutumidine as indicated (XX, R = He, and R = H), in accordance with structures previously obtained from x-ray analysis.

IT 17088-50-5 1814-26-1

L12 ANSWER 24 OF 28
ACCESSION NUMBER:
DOCUMENT NUMBER:
1967:517001 CAPLUS
67:117001
ACULUMINE and acutumidine, chlorine-containing alkaloids with a novel skeleton. I. X-ray analysis of acutumine
TOMITA, Masaon Okamoto, Yasukor Kikuchi, Tohrur Osaki, Kenjir Nishikawa, M.r. Kamiya, Kazuhide; Sasaki, Yukior Matoba, Katsuhide; Goto, Kakuji
Kyoto Univ., Kyoto, Japan
Tetrahedron Letters (1967), (25), 2421-4
CODEN: TELEATY ISSN: 0040-4039
Journal English
GI For diagram(s), see printed CA Issue.

UMENT TYPE: Journal GUAGE: English For diagram(s), see printed CA Issue. Isolation from Sinomenium cuttum and Menispermum dauricum gave the minor alkaloid acutumine (1), m. 238-40' (decomposition), (a]D -206' (CSHSM), and the N-nor base, acutumidine (11). N-Methylation of II, m. 239-41' (decomposition), [a]D -212' (CSHSM), showing close similarity to I in spectral properties, gave I. A 3-dimensional sharpende Patterson.function was calculated from 1459 independent data and from 14 tentative atomic positions; alternating applications of the least sqs. method and Fourier synthesis revealed the structure of I as shown (or its mirror image). Of the 14 atomic positions assumed at first, 4 were inadequate. Observed and calculated intensities of 29 pairs of reflections in the 1st and 2nd layers of Weissenberg photographs were compared from which the absolute configuration of the mol. was determined 17088-50-5 18145-26-1
RL: PRP (Properties) (Structure of) 17088-50-5 CABUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, club, so the structure of (IR,3'as,5s,7'as,9's)- (CA INDEX NAME)

Absolute stereochemistry.

18145-26-1 CAPLUS 1918-20-1 CAPLUS Spirc[3-cyclopentens-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (1R,3'as,5',7'as,9'5') (9CI) (CA NDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 23 OF 28 CAPLUS CUPYRIGHT 2007 ACS ON SIN (Continued) (structure of) 17088-50-5 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

Absolute stereochemistry.

18145-26-1 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano(lH]indole]-2,5'(4'H)-dione, 9'-chlor-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-, (lR,3'aS,5S,7'aS,9'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L12 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 1967:505042 CAPLUS
DOCUMENT NUMBER: 67:105042
TITLE: A region of biosynthesis

67:105042
A region of biosynthesis
Barton, Derek H. R.
Chemistry in Britain (1967), 3(8), 330-7
CODEN: CHMBAY: ISSN: 0009-3106 AUTHOR (S): SOURCE:

DOCUMENT TYPE:

CODEN: CHMBAY: ISSN: 0009-3106

MENT TYPE: Journal
UNGE: English
The developing interest in the biosynthesis of organic compds. is discussed, particularly in terms of reagent variation and its effect on specifically designed phenolic mols. The derivation of the structure of acutumine from phenolic coupling followed by further degradation is reviewed. Work previously described on the biosynthesis of sinomenine and Erythrina alkaloids (CA 67: 32851c) is also discussed. 38 references.

RI: PRP (Proparation)

17088-50-5
RL: PRP (Properties)
(atructure of, determination of)
17088-50-5 CAPUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

## Absolute stereochemistry.

L12 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1961:100140 CAPLUS DOCUMENT NUMBER: 55:100140 CAPLUS 55:100140 CAPLUS 55:18893d-e

ONIGINAL REFERENCE NO.: 55:1893d-e
Alkaloids of Menisperum dahuricum
Alkaloids:

Trudy Vsasoyuz. Nauch.-Issledovatel. Inst. Lekarstv. i
Aromat. Rast. (1959), (No. 11), 51-64
From Referat. Zhur. Khim., Biol. Khim. 1961, Abstr.
No. 6560.

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Two alkaloids were isolated from M. dahuricum: sinomenine, C19H2304N m.
161-2' (EELOM) and 180-1' (EICH) [2020 - 78, 9')
[EECH]) and acutumine. C2CH2708N m. 240-1' (EICH Et acetate 1:1)
[a] 200 - 120 (pyridine). Sinomenine was isolated from the total
alkaloids by Et acetate eccyptin. The root of the plant contained more
alkaloids than any other part. All parts contained a maximum of alkaloids
during bud formation and blooming.

[Trom Menisperum dauricum)
I 17088-50-5 CAPLUS
Spire[3-cyclopentene-1,10'-(3a,7a)propano[H]indole]-2.5' (4'H)-dional

17088-50-5 CAPLUS Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dlhydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

# Absolute stereochemistry.

L12 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 1957:454324 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 67:54324 CAPLUS

offselds
Characterization of acutumine
Goto, Kakuji: Tomita, Masao: Okamoto, Yasuko; Sasaki,
Yoshio: Matoba, Katsuhide
Proceedings of the Japan Academy (1966), 42(10), AUTHOR (S) :

SOURCE:

1181-4 CODEN: PJACAW; ISSN: 0021-4280

DOCUMENT TYPE: LANGUAGE:

Il81-4

CODEN: PJACAW, ISSN: 0021-4280

JUNENT TYPE: Journal

A revised mol. formula, C19H24NO6C1, is presented for acutumine (I), [pKa

5.3, m. 238-40', [a]150-206' (c 0.69, C5H5N)]. The

presence of C1 in I was proved by mass spectra and combustion data;

however, attempts to remove it by Ag20, LiAlH4, or catalytic

hydrogenolysis were unsuccessful. Acetylation with Ac20-C6H5N gave a

monoacetylated acutumine (II), m. 162-4' Oxidation of I with MnO2

gave oily dehydroacutumine with formation of a new carbonyl group and the

disappearance of the >CH0H proton group. I afforded a monoxine, m.

213', which no longer shows ir absorption at 1670 cm.-1, indicative

of one carbonyl group in I. Reduction of II with NaEH4 gave three products,

A, B, and C. A is shown by ir to have acetoxyl and hydroxyl groups, and

to lack the carbonyl group, Oxidation of A with MnO2 gave II. Acetylation

of A with Ac20-C5H5N afforded a diacetate, m. 149-52'. The

products B and C show the absence of both the acetoxy and the carbonyl

band at 1670 cm.-1 in the ir. Hydrogenation of II with LiAlH4

resulted in demethoxylation and reduction of the carbonyl group to give a

product m. 136-7'. Acetylation of this product with Ac20-C6H5N

gave a diacetate, m. 138-42''. Oxidation of the reduction product with

MnO2 gave a dehydro product, m. 166-9'. Reaction of I with

Pb(OAc)4 gave, as a major product, a CH0-containing compound

17088-50-5

RL: PRP (Properties)

17088-50-5
RL: PRP (Properties)
(properties of)
17088-50-5 CAPLUS
Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione,
9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-,
(1R,3'aS,5S,7'aS,9'S)- (CA INDEX NAME)

L12 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1930:7549 CAPLUS DOCUMENT NUMBER: 24:7549 CAPLUS L1TLE: Sinomenine and disinomenine. ID

Sinomenine and disinomenine. IX. Acutumine and

sinactine

AUTHOR (S): SOURCE: Sinactine Goto, Kakuji; Sudzuki, Hideo Bulletin of the Chemical Society of Japan (1929), 4, 220-4 CODEN: BCSJA8; ISSN: 0009-2673

220-4

CODIN: BCSJA0, ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 24, 122. Acutumine and sinactine are 2 alkaloids recently isolated from the root of Sinomenium acutum Rehd at Wills. Acutumine has the mol. formula C20H27NO8 or C21H27NO8. Its absorption spectrum resembles that of narccine. It m. 199-200'. Its HCl salt shows [a] D60.20'. The mol. contains 30Ms, 1CO, 1CO2H, 1NMs and no phenolic OH groups. Sinactine m. 174'. Its HCl salt decomps. at 272', its Au double salt is amorphous, its Pt double salt, m. 245-7'. In CHCl3, [a] D = -312'. The mol. formula is C19H21NO4, with 20Ms, 1 methylenedioxy, no NMs and no phenolic OH groups. The absorption spectrum almost coincides with that of laudanosine.

IT 17088-50-59, Acutumine RL: PREP (Preparation)
(preparation of)
NN 17088-50-5 CAPUS

Spiro[3-cyclopentene-1,10'-[3a,7a]propano[1H]indole]-2,5'(4'H)-dione, 9'-chloro-2',3'-dihydro-5-hydroxy-4,6',7'-trimethoxy-1'-methyl-, (1R,3'as,5s,7's)-5) - (CA INDEX NAME)

# Absolute stereochemistry.